

Isobutyric anhydride  
97-72-3 | DTXSID7026609

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 2.90

Global applicability domain: Inside

Local applicability domain index: 5.41e-01

Confidence level: 8.00e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Paraldehyde</div> <div>Measured: 3.02</div> <div>Predicted: 2.77</div>	<div>Image not found</div> <div>2-Isopropyl-6-methyl-4-pyrimidone</div> <div>Measured: 1.82</div> <div>Predicted: 2.23</div>	<div>Image not found</div> <div>O,O-Diethyl dithiophosphate</div> <div>Measured: 5.01</div> <div>Predicted: 5.43</div>
<div>Image not found</div> <div>Dimethoate</div> <div>Measured: 1.58</div> <div>Predicted: 1.88</div>	<div>Image not found</div> <div>2,2-Bis(bromomethyl)-1,3-propanediol</div> <div>Measured: 4.79</div> <div>Predicted: 3.35</div>	